Decyl methyl sulfide

Other names:	1-(Methylsulfanyl)decane
	2-Thiadodecane
	Decane, 1-(methylthio)-
	decyl methyl sulphide
	n-Decyl methyl sulfide
Inchi:	InChI=1S/C11H24S/c1-3-4-5-6-7-8-9-10-11-12-2/h3-11H2,1-2H3
InchiKey:	HKGUUZAACYBIID-UHFFFAOYSA-N
Formula:	C11H24S
SMILES:	CCCCCCCCCCSC
Mol. weight [g/mol]:	188.37
CAS:	22438-39-7

Physical Properties

Property code	Value	Unit	Source
gf	74.86	kJ/mol	Joback Method
hf	-228.50	kJ/mol	Joback Method
hfus	28.38	kJ/mol	Joback Method
hvap	46.90	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	4.490		Crippen Method
mcvol	182.200	ml/mol	McGowan Method
pc	1963.07	kPa	Joback Method
rinpol	1419.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1419.00		NIST Webbook
ripol	1656.00		NIST Webbook
tb	519.86	K	Joback Method
tc	700.00	K	Joback Method
tf	248.13	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	423.34	J/mol×K	519.86	Joback Method
cpg	439.87	J/mol×K	549.88	Joback Method
cpg	455.71	J/mol×K	579.91	Joback Method
cpg	470.88	J/mol×K	609.93	Joback Method
cpg	485.39	J/mol×K	639.95	Joback Method
cpg	499.25	J/mol×K	669.98	Joback Method
cpg	512.48	J/mol×K	700.00	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	398.20	K	1.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62022e+01
Coeff. B	-4.87498e+03
Coeff. C	-8.57270e+01
Temperature range (K), min.	392.05
Temperature range (K), max.	533.35

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22438397&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume